Author Index to Volume 165

Adamowicz, L., NNO–HCN complex. Ab initio calculations with the coupled cluster method and first-order correlation orbitals 165 (1992) 281
Aizpiri, A.G., F. Monroy, C. Del Campo, R.G. Rubio and M. Díaz Peña, Range of simple scaling and critical amplitudes near a LCST. The 2-butoxyethanol + water system 165 (1992) 31
Andrews, D.L. and A.M. Bittner, Selection rules for bimolecular photoabsorption 165 (1992) 1
Arikawa, T., see T. Sato 165 (1992) 173
Armentrout, P.B., see S. Niles 165 (1992) 143

Baranyai, A., see I. Borzsák 165 (1992) 227
Basilevsky, M.V. and G.E. Chudinov, On the role of medium electrons in the outer-sphere electron transfer reactions 165 (1992) 213
Bittner, A.M., see D.L. Andrews 165 (1992) 1
Bitto, H. and P.R. Willmott, The dynamics and its power dependence of $S_1(^1B_{3u})$ pyrazine studied with transform-limited nanosecond laser pulses 165 (1992) 113
Boiden Pedersen, J., L.I. Lolle and J.S. Jørgensen, An optimal numerical solution of diffusional recombination problems 165 (1992) 339
Borzsák, I. and A. Baranyai, On the convergence of Green's entropy expansion 165 (1992) 227
Brion, C.E., see P. Duffy 165 (1992) 183
Bruna, P.J. and F. Grein, Ab initio study of the vertical spectrum and ionization potentials of silanethione (H_2SiS) 165 (1992) 265

Cardini, G., see E. Venuti 165 (1992) 313
Casida, M.E., see P. Duffy 165 (1992) 183
Castellucci, E., see E. Venuti 165 (1992) 313
Chandra, A.K., see R. Sumathi 165 (1992) 257
Chauvistré, R., see G. Küper 165 (1992) 405
Chong, D.P., see P. Duffy 165 (1992) 183
Chudinov, G.E., see M.V. Basilevsky 165 (1992) 213
Clark, S.A.C., see P. Duffy 165 (1992) 183
Consalvo, D., D.H. Parker and J. Reuss, LIF-analysis on the $S_1 \leftarrow S_0$ transition of DABCO: "memory effect" and vibrational structure 165 (1992) 397

Davidson, E.R., see P. Duffy 165 (1992) 183
Del Campo, C., see A.G. Aizpiri 165 (1992) 31
Demes, H., see O. Shestakov 165 (1992) 415
Dereń, P., see B. Jassemnejad 165 (1992) 147
Dézarnaud-Dandine, C., see A. Sevin 165 (1992) 245
Díaz Peña, M., see A.G. Aizpiri 165 (1992) 31
Dickinson, A.S., see L.A. Viehland 165 (1992) 11

Author Index to Volume 165

Adamowicz, L., NNO–HCN complex. Ab initio calculations with the coupled cluster method and first-order correlation orbitals 165 (1992) 281
Aizpiri, A.G., F. Monroy, C. Del Campo, R.G. Rubio and M. Díaz Peña, Range of simple scaling and critical amplitudes near a LCST. The 2-butoxyethanol + water system 165 (1992) 31
Andrews, D.L. and A.M. Bittner, Selection rules for bimolecular photoabsorption 165 (1992) 1
Arikawa, T., see T. Sato 165 (1992) 173
Armentrout, P.B., see S. Niles 165 (1992) 143

Baranyai, A., see I. Borzsák 165 (1992) 227
Basilevsky, M.V. and G.E. Chudinov, On the role of medium electrons in the outer-sphere electron transfer reactions 165 (1992) 213
Bittner, A.M., see D.L. Andrews 165 (1992) 1
Bitto, H. and P.R. Willmott, The dynamics and its power dependence of $S_1(^1B_{3u})$ pyrazine studied with transform-limited nanosecond laser pulses 165 (1992) 113
Boiden Pedersen, J., L.I. Lolle and J.S. Jørgensen, An optimal numerical solution of diffusional recombination problems 165 (1992) 339
Borzsák, I. and A. Baranyai, On the convergence of Green's entropy expansion 165 (1992) 227
Brion, C.E., see P. Duffy 165 (1992) 183
Bruna, P.J. and F. Grein, Ab initio study of the vertical spectrum and ionization potentials of silanethione (H_2SiS) 165 (1992) 265

Cardini, G., see E. Venuti 165 (1992) 313
Casida, M.E., see P. Duffy 165 (1992) 183
Castellucci, E., see E. Venuti 165 (1992) 313
Chandra, A.K., see R. Sumathi 165 (1992) 257
Chauvistré, R., see G. Küper 165 (1992) 405
Chong, D.P., see P. Duffy 165 (1992) 183
Chudinov, G.E., see M.V. Basilevsky 165 (1992) 213
Clark, S.A.C., see P. Duffy 165 (1992) 183
Consalvo, D., D.H. Parker and J. Reuss, LIF-analysis on the $S_1 \leftarrow S_0$ transition of DABCO: "memory effect" and vibrational structure 165 (1992) 397

Davidson, E.R., see P. Duffy 165 (1992) 183
Del Campo, C., see A.G. Aizpiri 165 (1992) 31
Demes, H., see O. Shestakov 165 (1992) 415
Dereń, P., see B. Jassemnejad 165 (1992) 147
Dézarnaud-Dandine, C., see A. Sevin 165 (1992) 245
Díaz Peña, M., see A.G. Aizpiri 165 (1992) 31
Dickinson, A.S., see L.A. Viehland 165 (1992) 11

Di Stefano, G., M. Lenzi, G. Piciacchia and A. Ricci, Line intensities in the rotational branches of the PH($b\,^1\Sigma^+ v'=0 \rightarrow X\,^3\Sigma^- v''=0$) transition 165 (1992) 201
Doktorov, A.B., see V.A. Morozov 165 (1992) 297
Dolg, M., H. Stoll and H. Preuss, Ab initio pseudopotential study of YbH and YbF 165 (1992) 21
Duffy, P., S.A.C. Clark, C.E. Brion, M.E. Casida, D.P. Chong, E.R. Davidson and C. Maxwell, Electron momentum spectroscopy of the valence orbitals of acetylene: Quantitative comparisons using near Hartree–Fock limit and correlated wavefunctions 165 (1992) 183

Egorov, S.M., A.M. Pravilov and V.A. Skorokhodov, The very fast chemiluminescent reaction $I(5p^5\,^2P_{1/2}) + I(5p^5\,^2P_{3/2}) \rightarrow_{(M)} I_2(BO_u^+, v') \rightarrow I_2(XO_g^+, v') + h\nu$ 165 (1992) 371
Elofson, P.-A. and E. Ljungström, Stochastic simulation of $NO_2(X\,^2A_1) \rightarrow O(^3P_j) + NO(X\,^2\Pi_\Omega)$ photodissociation: rotational excitation of product NO 165 (1992) 323

Fink, E.H., see O. Shestakov 165 (1992) 415
Frick, F., see G. Küper 165 (1992) 405
Fujimoto, H., K. Kamiya, S. Tanaka, T. Mori, Y. Yamashita, H. Inokuchi and K. Seki, Electronic structure of bis[1,2,5]thiadiazolo-*p*-quinobis (1,3-dithiole) (BTQBT) studied by ultraviolet photoemission spectroscopy 165 (1992) 135

Gharavi, A., see G.L. McPherson 165 (1992) 361
Giménez, X., M. Moreno and J.M. Lluch, Ab initio study of the NH_3+OH reaction 165 (1992) 41
Grein, F., see P.J. Bruna 165 (1992) 265
Grice, S.T., see L.A. Viehland 165 (1992) 11
Grice, S.T., P.W. Harland and R.G.A.R. Maclagan, Calculation of the potential energy surface of Li^+–N_2 165 (1992) 73

Harland, P.W., see S.T. Grice 165 (1992) 73
Hartmann, E., see G. Küper 165 (1992) 405
Hormes, J., see G. Küper 165 (1992) 405

Inokuchi, H., see H. Fujimoto 165 (1992) 135

Jansen, M., see G. Küper 165 (1992) 405
Jaquet, R. and U. Schnupf, The S-matrix version of the Hulthén–Kohn variational principle for quantum scattering: comparison between conventional and finite element basis sets 165 (1992) 287
Jassemnejad, B., A. Suchocki, R.C. Powell, W. Stręk and P. Dereń, Optical spectroscopy and light-induced gratings in Cr^{3+} doped non-stoichiometric magnesium spinel 165 (1992) 147
Jørgensen, J.S., see J. Boiden Pedersen 165 (1992) 339

Kamiya, K., see H. Fujimoto 165 (1992) 135
Kasai, T., see H. Ohoyama 165 (1992) 155
Kawasaki, M., see T. Sato 165 (1992) 173
Kinugawa, T., see T. Sato 165 (1992) 173
Koptyug, A.V., see V.A. Morozov 165 (1992) 297

Küper, G., R. Chauvistré, J. Hormes, F. Frick, M. Jansen, B. Lüer and E. Hartmann, Phosphorus K shell photoabsorption spectra of the oxides P_4O_6, P_4O_{10}, $P(C_6H_5O)_3$ and $PO(C_6H_5O)_3$ 165 (1992) 405
Kuwata, K., see H. Ohoyama 165 (1992) 155

Lenzi, M., see G. Di Stefano 165 (1992) 201
Leroy, J.P., R. Wallace and H. Rabitz, A method for inverting curvilinear transformations of relevance in the quantum mechanical Hamiltonian describing *n*-body systems 165 (1992) 89
Ljungström, E., see P.-A. Elofson 165 (1992) 323
Lluch, J.M., see X. Giménez 165 (1992) 41
Lolle, L.I., see J. Boiden Pedersen 165 (1992) 339
Lowe, R.D., see J. Shen 165 (1992) 385
Lüer, B., see G. Küper 165 (1992) 405

Maciejewski, A., M. Szymanski and R.P. Steer, A dark, excited electronic state of thiophosgene in the near ultraviolet 165 (1992) 101
Maclagan, R.G.A.R., see L.A. Viehland 165 (1992) 11
Maclagan, R.G.A.R., see S.T. Grice 165 (1992) 73
Madsen, F., I. Terpager, K. Olskær and J. Spanget-Larsen, Ultraviolet–visible and infrared linear dichroism spectroscopy of 1,8-dihydroxy-9,10-anthraquinone aligned in stretched polyethylene 165 (1992) 351
Mai, J. and W. Von Niessen, A cellular automaton model with diffusion for a surface reaction system 165 (1992) 57
Mai, J. and W. Von Niessen, A cellular automaton model for the catalytic formation of NH_3 165 (1992) 65
Maxwell, C., see P. Duffy 165 (1992) 183
McPherson, G.L., A. Gharavi and S.L. Meyerson, Dynamics of up-conversion from simultaneously excited pairs of Er^{3+} ions in crystals of $CsMgCl_3$, $CsMgBr_3$ and $CsCdBr_3$ 165 (1992) 361
Meyerson, S.L., see G.L. McPherson 165 (1992) 361
Molin, Yu.N., see V.A. Morozov 165 (1992) 297
Monroy, F., see A.G. Aizpiri 165 (1992) 31
Moreno, M., see X. Giménez 165 (1992) 41
Mori, T., see H. Fujimoto 165 (1992) 135
Morozov, V.A., A.V. Koptyug, A.B. Doktorov and Yu.N. Molin, Dynamic theory of optically detected electron–nuclear double resonance of radical pairs (OD ENDOR) in liquid solutions 165 (1992) 297

Niles, S., P.B. Armentrout and C.A. Wight, Laser multiphoton dissociation and multiphoton ionization of $VOCl_3$ 165 (1992) 143

Ohasi, K., see H. Ohoyama 165 (1992) 155
Ohoyama, H., T. Kasai, K. Ohasi and K. Kuwata, Orientation-dependent CF_3 emission observed in the $Ar(^3P)+CF_3H \rightarrow CF_3^*(1E', 2A_2'')+H+Ar$ reaction 165 (1992) 155
Olskær, K., see F. Madsen 165 (1992) 351

Pandey, K.K., Electronic excitation transport, diffusion and trapping 165 (1992) 123
Parker, D.H., see D. Consalvo 165 (1992) 397
Piciacchia, G., see G. Di Stefano 165 (1992) 201

Powell, R.C., see B. Jassemnejad 165 (1992) 147
Pravilov, A.M., see S.M. Egorov 165 (1992) 371
Pravilov, A.M., see O. Shestakov 165 (1992) 415
Preuss, H., see M. Dolg 165 (1992) 21

Rabitz, H., see J.P. Leroy 165 (1992) 89
Reuss, J., see D. Consalvo 165 (1992) 397
Ricci, A., see G. Di Stefano 165 (1992) 201
Rubio, R.G., see A.G. Aizpiri 165 (1992) 31

Sato, T., T. Kinugawa, T. Arikawa and M. Kawasaki, Two-photon dissociation of SO_2 in the ultraviolet region 165 (1992) 173
Schnupf, U., see R. Jaquet 165 (1992) 287
Seki, K., see H. Fujimoto 165 (1992) 135
Sevin, A., C. Dézarnaud-Dandine and M. Tronc, A theoretical investigation of the adiabatic and diabatic behavior or the core-excited states of CH_3SH 165 (1992) 245
Shen, J., R.D. Lowe and R.D. Snook, A model for cw laser induced mode-mismatched dual-beam thermal lens spectrometry 165 (1992) 385
Shestakov, O., A.M. Pravilov, H. Demes and E.H. Fink, Radiative lifetime and quenching of the $A\,^2\Sigma^+$ and $X_2\,^2\Pi_{3/2}$ states of PbF 165 (1992) 415
Skorokhodov, V.A., see S.M. Egorov 165 (1992) 371
Snook, R.D., see J. Shen 165 (1992) 385
Spanget-Larsen, J., see F. Madsen 165 (1992) 351
Steer, R.P., see A. Maciejewski 165 (1992) 101
Stoll, H., see M. Dolg 165 (1992) 21
Stręk, W., see B. Jassemnejad 165 (1992) 147
Suchocki, A., see B. Jassemnejad 165 (1992) 147
Sumathi, R. and A.K. Chandra, Decomposition of formyl fluoride on the lowest triplet state surface 165 (1992) 257
Szymanski, M., see A. Maciejewski 165 (1992) 101

Tanaka, S., see H. Fujimoto 165 (1992) 135
Terpager, I., see F. Madsen 165 (1992) 351
Tronc, M., see A. Sevin 165 (1992) 245

Van Bladel, J.W.I., A. Van der Avoird and P.E.S. Wormer, The NH_3 umbrella motion in the Ar–NH_3 dimer 165 (1992) 47
Van der Avoird, A., see J.W.I. Van Bladel 165 (1992) 47
Venuti, E., G. Cardini and E. Castellucci, A molecular dynamics simulation of crystalline S_8 165 (1992) 313
Viehland, L.A., S.T. Grice, R.G.A.R. Maclagan and A.S. Dickinson, Transport coefficients for lithium ions in nitrogen gas: a test of the Li^+–N_2 interaction potential 165 (1992) 11
Vlad, M.O., Age–length distributions for branched chain processes 165 (1992) 231
Von Niessen, W., see J. Mai 165 (1992) 57
Von Niessen, W., see J. Mai 165 (1992) 65

Wallace, R., see J.P. Leroy 165 (1992) 89

Wight, C.A., see S. Niles 165 (1992) 143
Willmott, P.R., see H. Bitto 165 (1992) 113
Wormer, P.E.S., see J.W.I. Van Bladel 165 (1992) 47

Yamashita, Y., see H. Fujimoto 165 (1992) 135

Subject Index to Volume 165

Methods

Theoretical

Group theory and algebras
Selection rules for bimolecular photoabsorption, D.L. Andrews and A.M. Bittner 165 (1992) 1

Classical mechanics
Transport coefficients for lithium ions in nitrogen gas: a test of the Li^+–N_2 interaction potential, L.A. Viehland, S.T. Grice, R.G.A.R. Maclagan and A.S. Dickinson 165 (1992) 11

Many body and quasiparticle approaches
Electron momentum spectroscopy of the valence orbitals of acetylene: Quantitative comparisons using near Hartree–Fock limit and correlated wavefunctions, P. Duffy, S.A.C. Clark, C.E. Brion, M.E. Casida, D.P. Chong, E.R. Davidson and C. Maxwell 165 (1992) 183

Coupling schemes and perturbative treatments
Line intensities in the rotational branches of the PH($b\,^1\Sigma^+ v'=0 \rightarrow X\,^3\Sigma^- v''=0$) transition, G. Di Stefano, M. Lenzi, G. Piciacchia and A. Ricci 165 (1992) 201

Relativistic quantum mechanics
Ab initio pseudopotential study of YbH and YbF, M. Dolg, H. Stoll and H. Preuss 165 (1992) 21

Transport quantum mechanics
On the role of medium electrons in the outer-sphere electron transfer reactions, M.V. Basilevsky and G.E. Chudinov 165 (1992) 213

Equilibrium statistical mechanics
Range of simple scaling and critical amplitudes near a LCST. The 2-butoxyethanol + water system, A.G. Aizpiri, F. Monroy, C. Del Campo, R.G. Rubio and M. Díaz Peña 165 (1992) 31
On the convergence of Green's entropy expansion, I. Borzsák and A. Baranyai 165 (1992) 227

Statistical mechanics of stationary states
Age–length distributions for branched chain processes, M.O. Vlad 165 (1992) 231

Non-equilibrium thermodynamic and hydrodynamic theories
Age–length distributions for branched chain processes, M.O. Vlad 165 (1992) 231

Ab initio schemes for stationary properties
Ab initio pseudopotential study of YbH and YbF, M. Dolg, H. Stoll and H. Preuss 165 (1992) 21
Ab initio study of the NH_3+OH reaction, X. Giménez, M. Moreno and J.M. Lluch 165 (1992) 41
The NH_3 umbrella motion in the Ar–NH_3 dimer, J.W.I. Van Bladel, A. Van der Avoird and P.E.S. Wormer 165 (1992) 47
A theoretical investigation of the adiabatic and diabatic behavior or the core-excited states of CH_3SH, A. Sevin, C. Dézarnaud-Dandine and M. Tronc 165 (1992) 245
Decomposition of formyl fluoride on the lowest triplet state surface, R. Sumathi and A.K. Chandra 165 (1992) 257
Ab initio study of the vertical spectrum and ionization potentials of silanethione (H_2SiS), P.J. Bruna and F. Grein 165 (1992) 265
NNO–HCN complex. Ab initio calculations with the coupled cluster method and first-order correlation orbitals, L. Adamowicz 165 (1992) 281

Computational and simulation methods
Ab initio study of the NH_3+OH reaction, X. Giménez, M. Moreno and J.M. Lluch 165 (1992) 41
A cellular automaton model with diffusion for a surface reaction system, J. Mai and W. Von Niessen 165 (1992) 57
A cellular automaton model for the catalytic formation of NH_3, J. Mai and W. Von Niessen 165 (1992) 65
The S-matrix version of the Hulthén–Kohn variational principle for quantum scattering: comparison between conventional and finite element basis sets, R. Jaquet and U. Schnupf 165 (1992) 287
Dynamic theory of optically detected electron–nuclear double resonance of radical pairs (OD ENDOR) in liquid solutions, V.A. Morozov, A.V. Koptyug, A.B. Doktorov and Yu.N. Molin 165 (1992) 297
A molecular dynamics simulation of crystalline S_8, E. Venuti, G. Cardini and E. Castellucci 165 (1992) 313
Stochastic simulation of $NO_2(X^2A_1)\rightarrow O(^3P_J)+NO(X^2\Pi_\Omega)$ photodissociation: rotational excitation of product NO, P.-A. Elofson and E. Ljungström 165 (1992) 323
An optimal numerical solution of diffusional recombination problems, J. Boiden Pedersen, L.I. Lolle and J.S. Jørgensen 165 (1992) 339

Molecular dynamics and scattering theory
Calculation of the potential energy surface of Li^+–N_2, S.T. Grice, P.W. Harland and R.G.A.R. Maclagan 165 (1992) 73
A method for inverting curvilinear transformations of relevance in the quantum mechanical Hamiltonian describing *n*-body systems, J.P. Leroy, R. Wallace and H. Rabitz 165 (1992) 89
The S-matrix version of the Hulthén–Kohn variational principle for quantum scattering: comparison between conventional and finite element basis sets, R. Jaquet and U. Schnupf 165 (1992) 287

Experimental

Magnetic resonances
Dynamic theory of optically detected electron–nuclear double resonance of radical pairs (OD ENDOR) in liquid solutions, V.A. Morozov, A.V. Koptyug, A.B. Doktorov and Yu.N. Molin 165 (1992) 297

Infrared spectroscopy

Ultraviolet–visible and infrared linear dichroism spectroscopy of 1,8-dihydroxy-9,10-anthraquinone aligned in stretched polyethylene, F. Madsen, I. Terpager, K. Olskær and J. Spanget-Larsen 165 (1992) 351

Visible and UV spectroscopy

A dark, excited electronic state of thiophosgene in the near ultraviolet, A. Maciejewski, M. Szymanski and R.P. Steer 165 (1992) 101

Line intensities in the rotational branches of the PH($b\,^1\Sigma^+ v'=0 \rightarrow X\,^3\Sigma^- v''=0$) transition, G. Di Stefano, M. Lenzi, G. Piciacchia and A. Ricci 165 (1992) 201

Ultraviolet–visible and infrared linear dichroism spectroscopy of 1,8-dihydroxy-9,10-anthraquinone aligned in stretched polyethylene, F. Madsen, I. Terpager, K. Olskær and J. Spanget-Larsen 165 (1992) 351

Dynamics of up-conversion from simultaneously excited pairs of Er^{3+} ions in crystals of $CsMgCl_3$, $CsMgBr_3$ and $CsCdBr_3$, G.L. McPherson, A. Gharavi and S.L. Meyerson 165 (1992) 361

The very fast chemiluminescent reaction $I(5p^5\,^2P_{1/2}) + I(5p^5\,^2P_{3/2}) \rightarrow_{(M)} I_2(BO_u^+, v') \rightarrow I_2(XO_g^+, v') + h\nu$, S.M. Egorov, A.M. Pravilov and V.A. Skorokhodov 165 (1992) 371

A model for cw laser induced mode-mismatched dual-beam thermal lens spectrometry, J. Shen, R.D. Lowe and R.D. Snook 165 (1992) 385

Lif-analysis on the $S_1 \leftarrow S_0$ transition of DABCO: "memory effect" and vibrational structure, D. Consalvo, D.H. Parker and J. Reuss 165 (1992) 397

Fluorescence spectroscopy

A dark, excited electronic state of thiophosgene in the near ultraviolet, A. Maciejewski, M. Szymanski and R.P. Steer 165 (1992) 101

The dynamics and its power dependence of $S_1(^1B_{3u})$ pyrazine studied with transform-limited nanosecond laser pulses, H. Bitto and P.R. Willmott 165 (1992) 113

Electronic excitation transport, diffusion and trapping, K.K. Pandey 165 (1992) 123

Dynamics of up-conversion from simultaneously excited pairs of Er^{3+} ions in crystals of $CsMgCl_3$, $CsMgBr_3$ and $CsCdBr_3$, G.L. McPherson, A. Gharavi and S.L. Meyerson 165 (1992) 361

The very fast chemiluminescent reaction $I(5p^5\,^2P_{1/2}) + I(5p^5\,^2P_{3/2}) \rightarrow_{(M)} I_2(BO_u^+, v') \rightarrow I_2(XO_g^+, v') + h\nu$, S.M. Egorov, A.M. Pravilov and V.A. Skorokhodov 165 (1992) 371

Photoelectron and Auger spectroscopy

Electronic structure of bis[1,2,5]thiadiazolo-*p*-quinobis (1,3-dithiole) (BTQBT) studied by ultraviolet photoemission spectroscopy, H. Fujimoto, K. Kamiya, S. Tanaka, T. Mori, Y. Yamashita, H. Inokuchi and K. Seki 165 (1992) 135

X-ray spectroscopy

A theoretical investigation of the adiabatic and diabatic behavior or the core-excited states of CH_3SH, A. Sevin, C. Dézarnaud-Dandine and M. Tronc 165 (1992) 245

Phosphorus K shell photoabsorption spectra of the oxides P_4O_6, P_4O_{10}, $P(C_6H_5O)_3$ and $PO(C_6H_5O)_3$, G. Küper, R. Chauvistré, J. Hormes, F. Frick, M. Jansen, B. Lüer and E. Hartmann 165 (1992) 405

Electron impact spectroscopy

Electron momentum spectroscopy of the valence orbitals of acetylene: Quantitative comparisons using near Hartree–Fock limit and correlated wavefunctions, P. Duffy, S.A.C. Clark, C.E. Brion, M.E. Casida, D.P. Chong, E.R. Davidson and C. Maxwell 165 (1992) 183

Laser methods

Laser multiphoton dissociation and multiphoton ionization of $VOCl_3$, S. Niles, P.B. Armentrout and C.A. Wight 165 (1992) 143

A model for cw laser induced mode-mismatched dual-beam thermal lens spectrometry, J. Shen, R.D. Lowe and R.D. Snook 165 (1992) 385

Radiative lifetime and quenching of the $A\,^2\Sigma^+$ and $X_2\,^2\Pi_{3/2}$ states of PbF, O. Shestakov, A.M. Pravilov, H. Demes and E.H. Fink 165 (1992) 415

Non-linear optical spectroscopy

Selection rules for bimolecular photoabsorption, D.L. Andrews and A.M. Bittner 165 (1992) 1

Optical spectroscopy and light-induced gratings in Cr^{3+} doped non-stoichiometric magnesium spinel, B. Jassemnejad, A. Suchocki, R.C. Powell, W. Stręk and P. Dereń 165 (1992) 147

Synchrotron spectroscopies

Electronic structure of bis[1,2,5]thiadiazolo-*p*-quinobis (1,3-dithiole) (BTQBT) studied by ultraviolet photoemission spectroscopy, H. Fujimoto, K. Kamiya, S. Tanaka, T. Mori, Y. Yamashita, H. Inokuchi and K. Seki 165 (1992) 135

Phosphorus K shell photoabsorption spectra of the oxides P_4O_6, P_4O_{10}, $P(C_6H_5O)_3$ and $PO(C_6H_5O)_3$, G. Küper, R. Chauvistré, J. Hormes, F. Frick, M. Jansen, B. Lüer and E. Hartmann 165 (1992) 405

Coherent optical spectroscopy

A model for cw laser induced mode-mismatched dual-beam thermal lens spectrometry, J. Shen, R.D. Lowe and R.D. Snook 165 (1992) 385

Atomic and molecular beam techniques

Orientation-dependent CF_3 emission observed in the $Ar(^3P)+CF_3H \rightarrow CF_3^*(1E', 2A_2'')+H+Ar$ reaction, H. Ohoyama, T. Kasai, K. Ohasi and K. Kuwata 165 (1992) 155

Time-resolved experiments

The dynamics and its power dependence of $S_1(^1B_{3u})$ pyrazine studied with transform-limited nanosecond laser pulses, H. Bitto and P.R. Willmott 165 (1992) 113

Electronic excitation transport, diffusion and trapping, K.K. Pandey 165 (1992) 123

Optical spectroscopy and light-induced gratings in Cr^{3+} doped non-stoichiometric magnesium spinel, B. Jassemnejad, A. Suchocki, R.C. Powell, W. Stręk and P. Dereń 165 (1992) 147

Age–length distributions for branched chain processes, M.O. Vlad 165 (1992) 231

Dynamics of up-conversion from simultaneously excited pairs of Er^{3+} ions in crystals of $CsMgCl_3$, $CsMgBr_3$ and $CsCdBr_3$, G.L. McPherson, A. Gharavi and S.L. Meyerson 165 (1992) 361

The very fast chemiluminescent reaction $I(5p^5\,^2P_{1/2})+I(5p^5\,^2P_{3/2}) \rightarrow_{(M)} I_2(BO_u^+, v') \rightarrow I_2(XO_g^+, v')+h\nu$, S.M. Egorov, A.M. Pravilov and V.A. Skorokhodov 165 (1992) 371

Radiative lifetime and quenching of the $A\,^2\Sigma^+$ and $X_2\,^2\Pi_{3/2}$ states of PbF, O. Shestakov, A.M. Pravilov, H. Demes and E.H. Fink 165 (1992) 415

Mass spectrometry
Laser multiphoton dissociation and multiphoton ionization of $VOCl_3$, S. Niles, P.B. Armentrout and C.A. Wight 165 (1992) 143
Two-photon dissociation of SO_2 in the ultraviolet region, T. Sato, T. Kinugawa, T. Arikawa and M. Kawasaki 165 (1992) 173

Radiolysis
Age–length distributions for branched chain processes, M.O. Vlad 165 (1992) 231

Measurement of macroscopic variables
Range of simple scaling and critical amplitudes near a LCST. The 2-butoxyethanol+water system, A.G. Aizpiri, F. Monroy, C. Del Campo, R.G. Rubio and M. Díaz Peña 165 (1992) 31

Objects

Bulk systems

Gases
Transport coefficients for lithium ions in nitrogen gas: a test of the Li^+–N_2 interaction potential, L.A. Viehland, S.T. Grice, R.G.A.R. Maclagan and A.S. Dickinson 165 (1992) 11
Laser multiphoton dissociation and multiphoton ionization of $VOCl_3$, S. Niles, P.B. Armentrout and C.A. Wight 165 (1992) 143
Two-photon dissociation of SO_2 in the ultraviolet region, T. Sato, T. Kinugawa, T. Arikawa and M. Kawasaki 165 (1992) 173

Supersonic beams
The dynamics and its power dependence of $S_1(^1B_{3u})$ pyrazine studied with transform-limited nanosecond laser pulses, H. Bitto and P.R. Willmott 165 (1992) 113
LIF-analysis on the $S_1 \leftarrow S_0$ transition of DABCO: "memory effect" and vibrational structure, D. Consalvo, D.H. Parker and J. Reuss 165 (1992) 397

Liquids neat
On the convergence of Green's entropy expansion, I. Borzsák and A. Baranyai 165 (1992) 227

Liquids mixtures and solutions
Range of simple scaling and critical amplitudes near a LCST. The 2-butoxyethanol+water system, A.G. Aizpiri, F. Monroy, C. Del Campo, R.G. Rubio and M. Díaz Peña 165 (1992) 31
Electronic excitation transport, diffusion and trapping, K.K. Pandey 165 (1992) 123
On the role of medium electrons in the outer-sphere electron transfer reactions, M.V. Basilevsky and G.E. Chudinov 165 (1992) 213
A model for cw laser induced mode-mismatched dual-beam thermal lens spectrometry, J. Shen, R.D. Lowe and R.D. Snook 165 (1992) 385

Chrystals
Optical spectroscopy and light-induced gratings in Cr^{3+} doped non-stoichiometric magnesium spinel, B. Jassemnejad, A. Suchocki, R.C. Powell, W. Stręk and P. Dereń 165 (1992) 147

A molecular dynamics simulation of crystalline S_8, E. Venuti, G. Cardini and E. Castellucci 165 (1992) 313

–mixed

Dynamics of up-conversion from simultaneously excited pairs of Er^{3+} ions in crystals of $CsMgCl_3$, $CsMgBr_3$ and $CsCdBr_3$, G.L. McPherson, A. Gharavi and S.L. Meyerson 165 (1992) 361

Semiconductors

Electronic structure of bis[1,2,5]thiadiazolo-*p*-quinobis (1,3-dithiole) (BTQBT) studied by ultraviolet photoemission spectroscopy, H. Fujimoto, K. Kamiya, S. Tanaka, T. Mori, Y. Yamashita, H. Inokuchi and K. Seki 165 (1992) 135

Dielectrics

On the role of medium electrons in the outer-sphere electron transfer reactions, M.V. Basilevsky and G.E. Chudinov 165 (1992) 213

Microscopic systems

Molecules (neutral and ionic)

Transport coefficients for lithium ions in nitrogen gas: a test of the Li^+–N_2 interaction potential, L.A. Viehland, S.T. Grice, R.G.A.R. Maclagan and A.S. Dickinson 165 (1992) 11

Ab initio pseudopotential study of YbH and YbF, M. Dolg, H. Stoll and H. Preuss 165 (1992) 21

Decomposition of formyl fluoride on the lowest triplet state surface, R. Sumathi and A.K. Chandra 165 (1992) 257

The very fast chemiluminescent reaction $I(5p^5\,{}^2P_{1/2}) + I(5p^5\,{}^2P_{3/2}) \rightarrow_{(M)} I_2(BO_u^+, v') \rightarrow I_2(XO_g^+, v') + h\nu$, S.M. Egorov, A.M. Pravilov and V.A. Skorokhodov 165 (1992) 371

–diatomic

Ab initio pseudopotential study of YbH and YbF, M. Dolg, H. Stoll and H. Preuss 165 (1992) 21

Calculation of the potential energy surface of Li^+–N_2, S.T. Grice, P.W. Harland and R.G.A.R. Maclagan 165 (1992) 73

Line intensities in the rotational branches of the PH($b\,{}^1\Sigma^+ v'=0 \rightarrow X\,{}^3\Sigma^- v''=0$) transition, G. Di Stefano, M. Lenzi, G. Piciacchia and A. Ricci 165 (1992) 201

–small polyatomics

Ab initio study of the NH_3+OH reaction, X. Giménez, M. Moreno and J.M. Lluch 165 (1992) 41

Calculation of the potential energy surface of Li^+–N_2, S.T. Grice, P.W. Harland and R.G.A.R. Maclagan 165 (1992) 73

A method for inverting curvilinear transformations of relevance in the quantum mechanical Hamiltonian describing *n*-body systems, J.P. Leroy, R. Wallace and H. Rabitz 165 (1992) 89

A dark, excited electronic state of thiophosgene in the near ultraviolet, A. Maciejewski, M. Szymanski and R.P. Steer 165 (1992) 101

Two-photon dissociation of SO_2 in the ultraviolet region, T. Sato, T. Kinugawa, T. Arikawa and M. Kawasaki 165 (1992) 173

Electron momentum spectroscopy of the valence orbitals of acetylene: Quantitative comparisons using near Hartree–Fock limit and correlated wavefunctions, P. Duffy, S.A.C. Clark, C.E. Brion, M.E. Casida, D.P. Chong, E.R. Davidson and C. Maxwell 165 (1992) 183

A theoretical investigation of the adiabatic and diabatic behavior or the core-excited states of CH_3SH, A. Sevin, C. Dézarnaud-Dandine and M. Tronc 165 (1992) 245

Decomposition of formyl fluoride on the lowest triplet state surface, R. Sumathi and A.K. Chandra 165 (1992) 257
Ab initio study of the vertical spectrum and ionization potentials of silanethione (H_2SiS), P.J. Bruna and F. Grein 165 (1992) 265
Stochastic simulation of $NO_2(X\,^2A_1) \rightarrow O(^3P_j) + NO(X\,^2\Pi_\Omega)$ photodissociation: rotational excitation of product NO, P.-A. Elofson and E. Ljungström 165 (1992) 323
Phosphorus K shell photoabsorption spectra of the oxides P_4O_6, P_4O_{10}, $P(C_6H_5O)_3$ and $PO(C_6H_5O)_3$, G. Küper, R. Chauvistré, J. Hormes, F. Frick, M. Jansen, B. Lüer and E. Hartmann 165 (1992) 405

–aromatics
The dynamics and its power dependence of $S_1(^1B_{3u})$ pyrazine studied with transform-limited nanosecond laser pulses, H. Bitto and P.R. Willmott 165 (1992) 113
Electronic structure of bis[1,2,5]thiadiazolo-*p*-quinobis (1,3-dithiole) (BTQBT) studied by ultraviolet photoemission spectroscopy, H. Fujimoto, K. Kamiya, S. Tanaka, T. Mori, Y. Yamashita, H. Inokuchi and K. Seki 165 (1992) 135
Ultraviolet–visible and infrared linear dichroism spectroscopy of 1,8-dihydroxy-9,10-anthraquinone aligned in stretched polyethylene, F. Madsen, I. Terpager, K. Olskær and J. Spanget-Larsen 165 (1992) 351

–other large
Laser multiphoton dissociation and multiphoton ionization of $VOCl_3$, S. Niles, P.B. Armentrout and C.A. Wight 165 (1992) 143
LIF-analysis on the $S_1 \leftarrow S_0$ transition of DABCO: "memory effect" and vibrational structure, D. Consalvo, D.H. Parker and J. Reuss 165 (1992) 397

Molecular aggregates

–van der Waals molecules
The NH_3 umbrella motion in the Ar–NH_3 dimer, J.W.I. Van Bladel, A. Van der Avoird and P.E.S. Wormer 165 (1992) 47

–complexes
NNO–HCN complex. Ab initio calculations with the coupled cluster method and first-order correlation orbitals, L. Adamowicz 165 (1992) 281

Free radicals (including hydronium and muonium)
Ab initio study of the $NH_3 + OH$ reaction, X. Giménez, M. Moreno and J.M. Lluch 165 (1992) 41
Dynamic theory of optically detected electron–nuclear double resonance of radical pairs (OD ENDOR) in liquid solutions, V.A. Morozov, A.V. Koptyug, A.B. Doktorov and Yu.N. Molin 165 (1992) 297
Radiative lifetime and quenching of the $A\,^2\Sigma^+$ and $X_2\,^2\Pi_{3/2}$ states of PbF, O. Shestakov, A.M. Pravilov, H. Demes and E.H. Fink 165 (1992) 415

Defects and impurities
Optical spectroscopy and light-induced gratings in Cr^{3+} doped non-stoichiometric magnesium spinel, B. Jassemnejad, A. Suchocki, R.C. Powell, W. Stręk and P. Dereń 165 (1992) 147

Ions and charge carriers
On the role of medium electrons in the outer-sphere electron transfer reactions, M.V. Basilevsky and G.E. Chudinov 165 (1992) 213
Dynamic theory of optically detected electron–nuclear double resonance of radical pairs (OD ENDOR) in liquid solutions, V.A. Morozov, A.V. Koptyug, A.B. Doktorov and Yu.N. Molin 165 (1992) 297

Phenomena

Molecular structure
Phosphorus K shell photoabsorption spectra of the oxides P_4O_6, P_4O_{10}, $P(C_6H_5O)_3$ and $PO(C_6H_5O)_3$, G. Küper, R. Chauvistré, J. Hormes, F. Frick, M. Jansen, B. Lüer and E. Hartmann 165 (1992) 405

Vibrations and rotations of molecules
The NH_3 umbrella motion in the Ar–NH_3 dimer, J.W.I. Van Bladel, A. Van der Avoird and P.E.S. Wormer 165 (1992) 47
A method for inverting curvilinear transformations of relevance in the quantum mechanical Hamiltonian describing *n*-body systems, J.P. Leroy, R. Wallace and H. Rabitz 165 (1992) 89
Stochastic simulation of $NO_2(X\,^2A_1) \rightarrow O(^3P_j) + NO(X\,^2\Pi_\Omega)$ photodissociation: rotational excitation of product NO, P.-A. Elofson and E. Ljungström 165 (1992) 323
Ultraviolet–visible and infrared linear dichroism spectroscopy of 1,8-dihydroxy-9,10-anthraquinone aligned in stretched polyethylene, F. Madsen, I. Terpager, K. Olskær and J. Spanget-Larsen 165 (1992) 351
LIF-analysis on the $S_1 \leftarrow S_0$ transition of DABCO: "memory effect" and vibrational structure, D. Consalvo, D.H. Parker and J. Reuss 165 (1992) 397

Electronic structure and states
Ab initio pseudopotential study of YbH and YbF, M. Dolg, H. Stoll and H. Preuss 165 (1992) 21
A dark, excited electronic state of thiophosgene in the near ultraviolet, A. Maciejewski, M. Szymanski and R.P. Steer 165 (1992) 101
Electronic structure of bis[1,2,5]thiadiazolo-*p*-quinobis (1,3-dithiole) (BTQBT) studied by ultraviolet photoemission spectroscopy, H. Fujimoto, K. Kamiya, S. Tanaka, T. Mori, Y. Yamashita, H. Inokuchi and K. Seki 165 (1992) 135
A theoretical investigation of the adiabatic and diabatic behavior or the core-excited states of CH_3SH, A. Sevin, C. Dézarnaud-Dandine and M. Tronc 165 (1992) 245
Ab initio study of the vertical spectrum and ionization potentials of silanethione (H_2SiS), P.J. Bruna and F. Grein 165 (1992) 265
Ultraviolet–visible and infrared linear dichroism spectroscopy of 1,8-dihydroxy-9,10-anthraquinone aligned in stretched polyethylene , F. Madsen, I. Terpager, K. Olskær and J. Spanget-Larsen 165 (1992) 351
Lif-analysis on the $S_1 \leftarrow S_0$ transition of DABCO: "memory effect" and vibrational structure, D. Consalvo, D.H. Parker and J. Reuss 165 (1992) 397

Phosphorus K shell photoabsorption spectra of the oxides P_4O_6, P_4O_{10}, $P(C_6H_5O)_3$ and $PO(C_6H_5O)_3$, G. Küper, R. Chauvistré, J. Hormes, F. Frick, M. Jansen, B. Lüer and E. Hartmann 165 (1992) 405

Molecular interactions
Selection rules for bimolecular photoabsorption, D.L. Andrews and A.M. Bittner 165 (1992) 1
Transport coefficients for lithium ions in nitrogen gas: a test of the Li^+–N_2 interaction potential, L.A. Viehland, S.T. Grice, R.G.A.R. Maclagan and A.S. Dickinson 165 (1992) 11
The NH_3 umbrella motion in the Ar–NH_3 dimer, J.W.I. Van Bladel, A. Van der Avoird and P.E.S. Wormer 165 (1992) 47
Calculation of the potential energy surface of Li^+–N_2, S.T. Grice, P.W. Harland and R.G.A.R. Maclagan 165 (1992) 73

Spectral bandshapes and intensities
Line intensities in the rotational branches of the PH($b\,^1\Sigma^+ v'=0 \rightarrow X\,^3\Sigma^- v''=0$) transition, G. Di Stefano, M. Lenzi, G. Piciacchia and A. Ricci 165 (1992) 201
A molecular dynamics simulation of crystalline S_8, E. Venuti, G. Cardini and E. Castellucci 165 (1992) 313

Coupling of electronic and nuclear motion
Line intensities in the rotational branches of the PH($b\,^1\Sigma^+ v'=0 \rightarrow X\,^3\Sigma^- v''=0$) transition, G. Di Stefano, M. Lenzi, G. Piciacchia and A. Ricci 165 (1992) 201

Energy transfer processes
Electronic excitation transport, diffusion and trapping, K.K. Pandey 165 (1992) 123
Dynamics of up-conversion from simultaneously excited pairs of Er^{3+} ions in crystals of $CsMgCl_3$, $CsMgBr_3$ and $CsCdBr_3$, G.L. McPherson, A. Gharavi and S.L. Meyerson 165 (1992) 361
Radiative lifetime and quenching of the $A\,^2\Sigma^+$ and $X_2\,^2\Pi_{3/2}$ states of PbF, O. Shestakov, A.M. Pravilov, H. Demes and E.H. Fink 165 (1992) 415

Molecular photophysical processes
Selection rules for bimolecular photoabsorption, D.L. Andrews and A.M. Bittner 165 (1992) 1
A dark, excited electronic state of thiophosgene in the near ultraviolet, A. Maciejewski, M. Szymanski and R.P. Steer 165 (1992) 101
Laser multiphoton dissociation and multiphoton ionization of $VOCl_3$, S. Niles, P.B. Armentrout and C.A. Wight 165 (1992) 143

Intramolecular dynamics
The NH_3 umbrella motion in the Ar–NH_3 dimer, J.W.I. Van Bladel, A. Van der Avoird and P.E.S. Wormer 165 (1992) 47

–radiationless transitions
The dynamics and its power dependence of $S_1(^1B_{3u})$ pyrazine studied with transform-limited nanosecond laser pulses, H. Bitto and P.R. Willmott 165 (1992) 113
A model for cw laser induced mode-mismatched dual-beam thermal lens spectrometry, J. Shen, R.D. Lowe and R.D. Snook 165 (1992) 385

Luminescence spectra, yields and lifetimes
Radiative lifetime and quenching of the $A^2\Sigma^+$ and $X_2{}^2\Pi_{3/2}$ states of PbF, O. Shestakov, A.M. Pravilov, H. Demes and E.H. Fink 165 (1992) 415

Non-linear responses (including optical)
Optical spectroscopy and light-induced gratings in Cr^{3+} doped non-stoichiometric magnesium spinel, B. Jassemnejad, A. Suchocki, R.C. Powell, W. Stręk and P. Dereń 165 (1992) 147

Multiphoton phenomena
Selection rules for bimolecular photoabsorption, D.L. Andrews and A.M. Bittner 165 (1992) 1

Reactions (including dissociation)
Age–length distributions for branched chain processes, M.O. Vlad 165 (1992) 231
Decomposition of formyl fluoride on the lowest triplet state surface, R. Sumathi and A.K. Chandra 165 (1992) 257
The S-matrix version of the Hulthén–Kohn variational principle for quantum scattering: comparison between conventional and finite element basis sets, R. Jaquet and U. Schnupf 165 (1992) 287
An optimal numerical solution of diffusional recombination problems, J. Boiden Pedersen, L.I. Lolle and J.S. Jørgensen 165 (1992) 339
The very fast chemiluminescent reaction $I(5p^5\,{}^2P_{1/2})+I(5p^5\,{}^2P_{3/2})\rightarrow_{(M)}I_2(BO_u^+, v')\rightarrow I_2(XO_g^+, v')+h\nu$, S.M. Egorov, A.M. Pravilov and V.A. Skorokhodov 165 (1992) 371

–gas phase
Ab initio study of the NH_3+OH reaction, X. Giménez, M. Moreno and J.M. Lluch 165 (1992) 41
Orientation-dependent CF_3 emission observed in the $Ar(^3P)+CF_3H\rightarrow CF_3^*(1E', 2A_2'')+H+Ar$ reaction, H. Ohoyama, T. Kasai, K. Ohasi and K. Kuwata 165 (1992) 155

–condensed phase
Electronic excitation transport, diffusion and trapping, K.K. Pandey 165 (1992) 123
On the role of medium electrons in the outer-sphere electron transfer reactions, M.V. Basilevsky and G.E. Chudinov 165 (1992) 213

–photochemical
Two-photon dissociation of SO_2 in the ultraviolet region, T. Sato, T. Kinugawa, T. Arikawa and M. Kawasaki 165 (1992) 173
Decomposition of formyl fluoride on the lowest triplet state surface, R. Sumathi and A.K. Chandra 165 (1992) 257
Stochastic simulation of $NO_2(X\,{}^2A_1)\rightarrow O(^3P_j)+NO(X\,{}^2\Pi_\Omega)$ photodissociation: rotational excitation of product NO, P.-A. Elofson and E. Ljungström 165 (1992) 323

Ionization (including Rydberg states)
Ab initio study of the vertical spectrum and ionization potentials of silanethione (H_2SiS), P.J. Bruna and F. Grein 165 (1992) 265

Molecular motion (including diffusive)
An optimal numerical solution of diffusional recombination problems, J. Boiden Pedersen, L.I. Lolle and J.S. Jørgensen 165 (1992) 339

Collective motion and excitations
A molecular dynamics simulation of crystalline S_8, E. Venuti, G. Cardini and E. Castellucci 165 (1992) 313

Surface effects and catalysis
A cellular automaton model with diffusion for a surface reaction system, J. Mai and W. Von Niessen 165 (1992) 57
A cellular automaton model for the catalytic formation of NH_3, J. Mai and W. Von Niessen 165 (1992) 65

Thermodynamic and transport properties
Transport coefficients for lithium ions in nitrogen gas: a test of the Li^+–N_2 interaction potential, L.A. Viehland, S.T. Grice, R.G.A.R. Maclagan and A.S. Dickinson 165 (1992) 11
On the convergence of Green's entropy expansion, I. Borzsák and A. Baranyai 165 (1992) 227

Structure of solids and liquids
A molecular dynamics simulation of crystalline S_8, E. Venuti, G. Cardini and E. Castellucci 165 (1992) 313

Critical phenomena
Range of simple scaling and critical amplitudes near a LCST. The 2-butoxyethanol + water system, A.G. Aizpiri, F. Monroy, C. Del Campo, R.G. Rubio and M. Díaz Peña 165 (1992) 31

Phase transitions
A cellular automaton model with diffusion for a surface reaction system, J. Mai and W. Von Niessen 165 (1992) 57
A cellular automaton model for the catalytic formation of NH_3, J. Mai and W. Von Niessen 165 (1992) 65